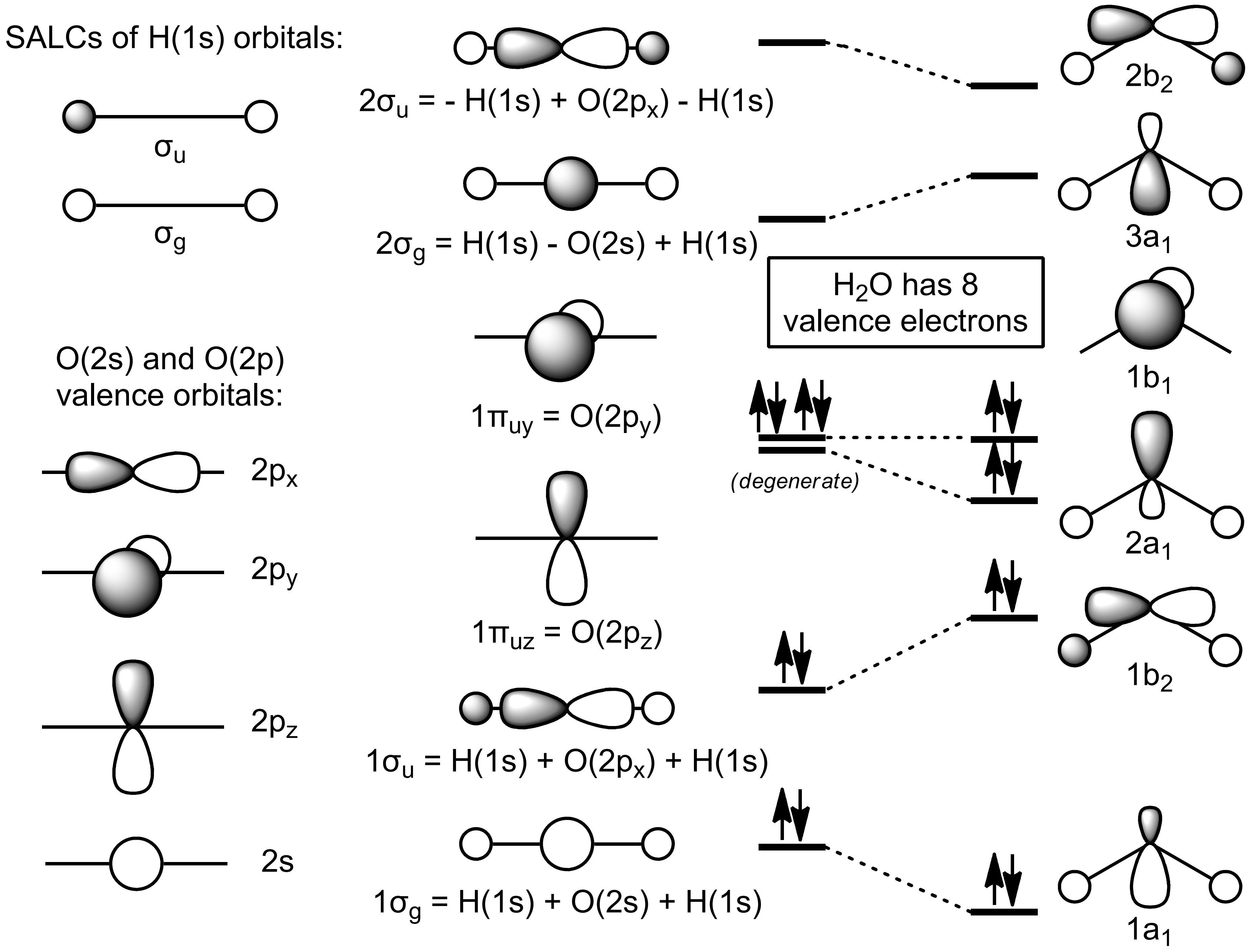
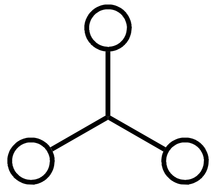
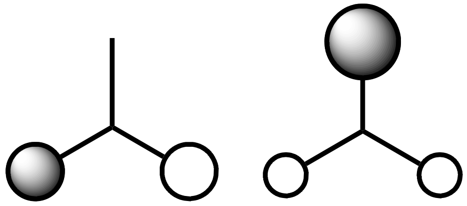

SALCs of H(1s) orbitals:
σ_u
σ_g
O(2s) and O(2p) valence orbitals:
$2p_x$
$2p_y$
$2p_z$
2s
$2\sigma_u$ = - H(1s) + O($2p_x$) - H(1s)
$2\sigma_g$ = H(1s) - O(2s) + H(1s)
$1\pi_{uy}$ = O($2p_y$)
$1\pi_{uz}$ = O($2p_z$)
$1\sigma_u$ = H(1s) + O($2p_x$) + H(1s)
$1\sigma_g$ = H(1s) + O(2s) + H(1s)
H_2O has 8 valence electrons
(degenerate)
$2b_2$
$3a_1$
$1b_1$
$2a_1$
$1b_2$
$1a_1$

SALC stands for symmetry adapted linear combination. These are the sets of orbitals that are of the right symmetry for constructing an MO diagram

The **Walsh diagram** (orbital diagram plotting orbital energy against a change in a geometric parameter) of water indicates a the favorable energy change as $1\pi_{uz}$ becomes $2a_1$; this explains the bent geometry of H_2O and other 8 electron AH_2 species.

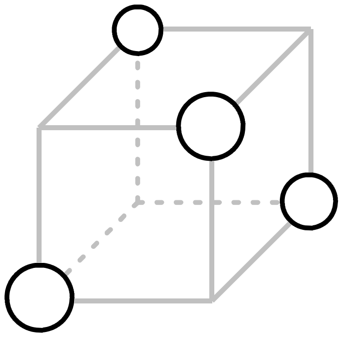


a_1 orbitals

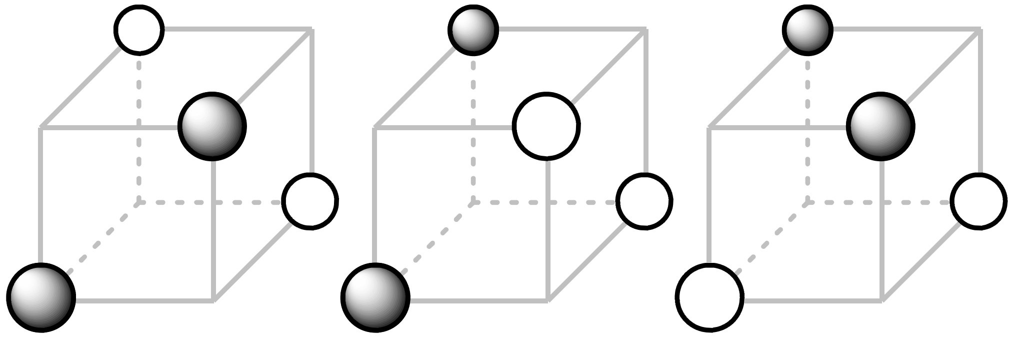


two sets of e orbitals

Exercise: What does the Walsh diagram say about the geometries of BeH_2 and CH_2?
Exercise: How do the p orbitals of C in CH_4 interact with the H-based SALCs?
Harder exercise: Construct a Walsh diagram for AH_3; show why NH_3 is pyramidal.



a_1 orbitals



three sets of t_2 orbitals